

Hessian Free Optimization

ritchie huang

2019-09-09

Contents

1	Background	2
2	Conjugate Gradient	2
2.1	Prerequisite	2

1 Background

we can get approximation of $f(x)$ in second-order Tylor expansion:

$$f(x + \Delta x) \approx f(x) + \nabla f(x)^T \Delta x + \Delta x^T H(f) \Delta x \quad (1)$$

2 Conjugate Gradient

Suppose we define function as bellow:

$$f(x) = \frac{1}{2}x^T A x + b^T x + c. \quad x, b, c \in \mathbb{R}^n \quad (2)$$

where $A^T = A$, that's say A is symmetric.

2.1 Prerequisite

Taking gradient of f , we obtain:

$$\nabla f(x) = Ax + b \quad (3)$$

the direction of gradient is the direction in which the function rises fastest.

If we hope to minimize our function, we can then update x by:

$$x = x - \alpha \nabla f(x) \quad (4)$$

where α is called step-size (may be learning rate), we perform a line search to find the best α when the direction $d_0 = \nabla f(x)$ is given.

Note that choosing the best α is equivalent to minimize the following function:

$$\begin{aligned} g(\alpha) &= f(x_0 + \alpha d_0) \\ &= \frac{1}{2}(x_0 + \alpha d_0)^T A (x_0 + \alpha d_0) + b^T (x_0 + \alpha d_0) + c \\ &= \frac{1}{2}\alpha^2 d_0^T A d_0 + d_0^T (Ax_0 + b)\alpha + \left(\frac{1}{2}x_0^T A x_0 + b^T x_0 + c \right) \end{aligned} \quad (5)$$

More generally, when we update x_i iteratively, since $g(\alpha)$ is a quadratic function in α , it has a unique global minimum or maximum. Assume this function has a global minimum where $g'(\alpha) = 0$:

$$g'(\alpha) = \alpha(d_i^T A d_i) + d_i^T (Ax_i + b) = 0 \quad (6)$$

Solving the equation above, we obtain:

$$\alpha = -\frac{d_i^T(Ax_i + b)}{d_i^T Ad_i} \quad (7)$$

Thus, we can update x_1 using x_0 and α in the iterative algorithm:

$$x_1 = x_0 - \alpha \nabla f(x_0) \quad (8)$$

However, it's subtle that each α_i is related to $d_i = -\nabla f(x_i)$, when we are going to update x_{i+1} , we may ruin our update from previous iteration. Therefore, we need to rectify direction d_{i+1} , which is conjugate to d_i .

$$d_{i+1} = -\nabla f(x_{i+1}) + \beta_i d_i \quad (9)$$

But, what's β_i ? We can derive it from the conjugacy between d_{i+1} and d_i .

We define vector x and y to be conjugate w.r.t a semi-definite matrix A if $x^T Ay = 0$.

We obtain that:

$$\begin{aligned} d_{i+1}^T Ad_i &= 0 \\ &= (-\nabla f(x_{i+1}) + \beta_i d_i)^T Ad_i \\ &= -\nabla f(x_{i+1})^T Ad_i + \beta_i d_i^T Ad_i \end{aligned} \quad (10)$$

Solve the equation above:

$$\beta_i = \frac{\nabla f(x_{i+1})^T Ad_i}{d_i^T Ad_i} \quad (11)$$